EUROfusion

“THEORY, SIMULATION, VERIFICATION AND VALIDATION”

TSVV TASK 7: PLASMA-WALL INTERACTION IN DEMO

pre-KICK-OFF INFORMATION MEETING

D. MATVEEV | 09.04.2021

JSI

UNIVERSITY OF HELSINKI

KTH VETENSKAP OCH KONST

cea

Université Sorbonne Paris Nord

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IPP

JÜLICH Forschungszentrum

OUTLINE

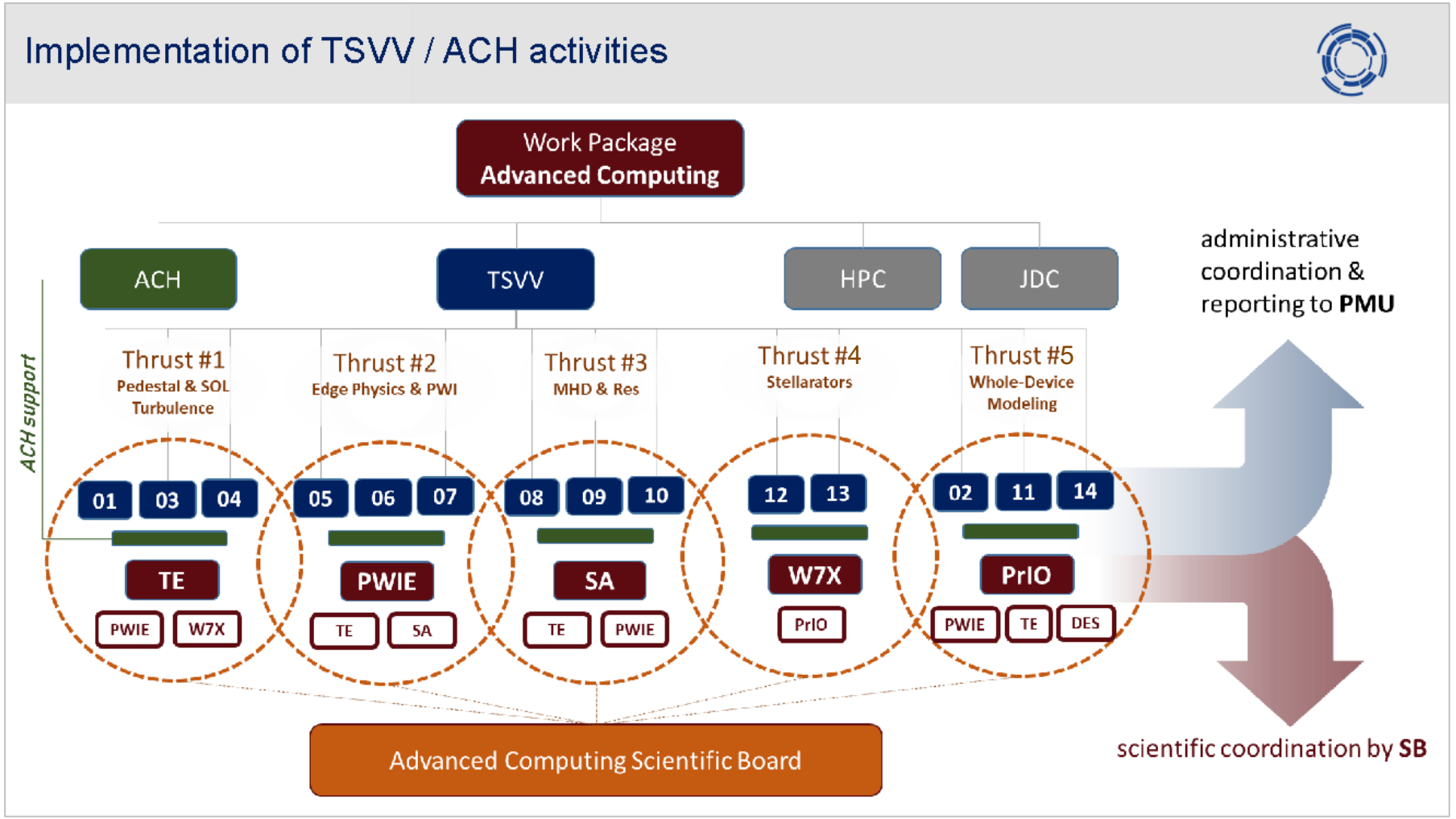
- Organizational placement of TSVVs
- Task commitments
- Objectives, milestones and deliverables
- Subtasks, timeline and communication
- ACH support
- Marconi 5th cycle
- Online resources
- Kick-Off meeting(s)

Organizational placement of TSVVs

- Each TSVV Task is treated organizationally as a project under the respective TSVV PI
- Collectively TSVVs are placed within the **WP "Advanced Computation"**, together with ACHs
- Primary partner WPs have been identified for each TSVV to ensure work integration **(WPPWIE)**
- Each milestone and deliverable for TSVVs will need to be formulated jointly with respective WPs
- TSVVs report to the E-TASC SB, where the PLs and TFLs are represented
- For the alignment of the daily work with the needs of the WPs, a number of specific scientific panels (including the PLs and TSVV PIs) will be established – **Thrusts (see next slide)**
- Regarding publications and use of data, all relevant PLs/TFLs are always to be kept informed
- Clearance of papers from TSVVs must always include, besides the PI, at least one WP leader

Organizational placement of TSVVs

(this slide will be shown at the TSVV/ACH Kick-Off Meeting on 23.04.2021)



Thrust #2:
Edge Physics & PWI

Facilitator:

S. Brezinsek [WPPWIE]

Involving:

D. Borodin [TSVV5]
G. Ciraolo [TSVV6]
D. Matveev [TSVV7]
A. Alonso [WPW7X]
C. Sozzi [WPSA]
M. Wischmeier [WPTE]
B. Braams [AC SB]
D. Tskhakaya [AC SB]

Task commitments

Team member	R.U.	Commitment (PM)				
		2021	2022	2023	2024	2025
Dmitry Matveev	FZJ	9	6	6	6	6
Juri Romazanov		0	4	6	6	6
Sebastian Rode		9	9	6	6	6
NN		6	6	6	6	6
Michael Komm	IPP.CR	1	1	1	1	1
Aleš Podolník		6	6	6	6	6
David Tskhakaya		0	0	0	0	0
Jernej Kovačič	JSI	6	6	6	6	6
Fredric Granberg	VTT	0	6	6	6	6
Alvaro Lopez-Cazalilla		6	0	0	0	0
Jonathan Mougenot	CEA	5	5	5	5	5
Yann Charles		5	5	5	5	5
Christian Grisolia		6	6	6	6	6
Etienne Hodille		6	6	6	6	6
Rémi Delaporte-Mathurin		6	6	0	0	0
Klaus Schmid	IPP	6	6	6	0	6
Udo von Toussaint		0	12	12	12	12
Svetlana Ratynskaia	VR	6	6	6	6	6
Panagiotis Tolias		6	6	0	6	6
Ladislas Vignitchouk		6	6	6	6	6
Emil Thorén		0	0	6	0	0
Total (w/o contributions covered by other means)		**88**	**101**	**100**	**94**	**100**

Research unit	*Commitment (PM)*				
	2021	*2022*	*2023*	*2024*	*2025*
ACH	32	19	20	26	20

covered by other means

- The budget for TSVV in k€ is based on the average European salary
- Real costs of the ppy depend on the real salary rate per RU
- Real costs summed up can be above the allocated budget for the TSVV
- Start of the project on the 1st of April means (possibly, but not necessarily) up to 3 months per person reduction in commitments for 2021 to (at least partly) compensate for the difference

Objectives

- Assessment of steady-state W erosion rates for first wall and divertor
- Mapping of preferential W re/co-deposition locations
- Assessment of dust mobilization from likely dust production sites
  (dust survival rates and dust accumulation maps)
- Assessment of PFC response to transients: melting and splashing
  (melt-stability, likelihood of splashing, droplet-to-dust conversion rates)
- Assessment of W erosion rates for locations affected by transients
- Assessment of tritium in-vessel inventory
  (co-deposition, bulk retention with He-induced and neutron damage)

Milestones (2021)

- In the absence of a DEMO-specific plasma background, the work in TSVV7 in 2021 will concentrate to a large extent on the adaptation of available ITER plasma backgrounds to DEMO, respective scoping PIC and dust simulations, and identification of HPC optimization and IMAS integration solutions for the codes.
- In particular, scoping PIC simulations will assess the characteristics of the plasma sheath with the focus on data for erosion simulations with ERO2.0.
- Another part of the project will focus on the code development and validation for retention studies, namely on the thermo-migration and material interface models in respective codes.
- MD simulations of erosion of H supersaturated W will be set up and provide first results linking retention with erosion.
- The following two major milestones are envisaged:
  - Available ITER plasma backgrounds are adapted to DEMO, serve for first PIC and dust transport scoping simulations, and are ready to be used in ERO2.0.
  - Thermo-migration and interface models are implemented and validated in retention codes (TESSIM-X and FESTIM) with identified common test cases.

Milestones (2021)

Year 1: ITER-like plasma case	
M1.1	SOLPS-ITER steady-state plasma background (ITER plasma) is adapted to DEMO, post-processed for ERO2.0 and MIGRAINe, relevant data are extracted for PIC simulations.
M1.2	Scoping PIC simulations are performed to assess the characteristics of the plasma sheath and resulting impact angles and energies in steady state.
M1.3	Intermediate results on erosion of H supersaturated W from MD simulations are reported.
M1.4	MIGRAINe scoping dust transport simulations with ITER-like ramp-up and steady state plasma profiles are performed.
M1.5	Thermo-migration is implemented in TESSIM-X and validated.
M1.6	Validation of the interface model of FESTIM is completed.
M1.7	Common test cases for retention modelling are identified.
M1.8	HPC optimization requirements for the codes are identified, the respective work initiated.

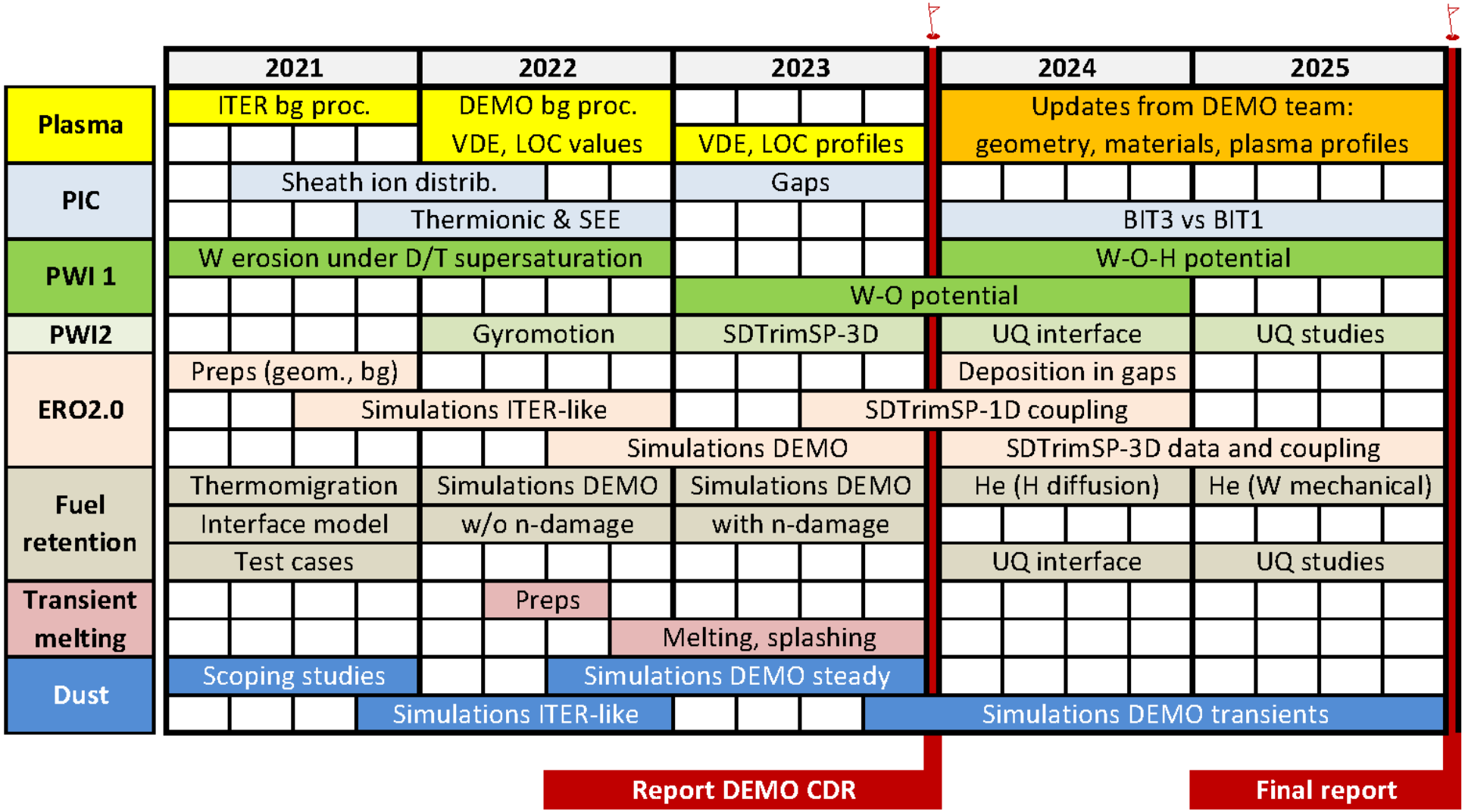
Sub-tasks and deliverables

Sub-Task		*Sub-Task Leader*	*Contribution to deliverables*
ST1	PIC-1 (BIT)	Jernej Kovačič	D1, D10, D14
ST2	PIC-2 (SPICE)	Aleš Podolník	D2, D4, D5, D14
ST3	PWI-1 (MD)	Fredric Granberg	D12, D13, D14
ST4	PWI-2 (SDTrimSP)	Udo von Toussaint	D4, D11, D14
ST5	ERO2.0 modelling	Juri Romazanov	D1, D2, D4, D14
ST6	Fuel retention	Jonathan Mougenot	D8, D9, D14
ST7	Uncertainty quantification	Udo von Toussaint	D9, D11, D14
ST8	Transient melting	Svetlana Ratynskaia	D3, D5, D14
ST9	Dust	Svetlana Ratynskaia	D5, D6, D7, D14

List of deliverables

D1	Steady state W erosion rates at DEMO first wall and divertor.
D2	Location mapping for net (co-)deposition and impurity sources from the wall.
D3	Large-scale surface modifications due to melting and melt-motion induced by transients.
D4	Assessment of surface roughness and lifetime of PFC affected by transients.
D5	Stability of melt layers during transients. Droplet sizes and speeds in case of splashing.
D6	A catalog of representative cases for dust (re-)mobilization conditions.
D7	Dust survival rates, inventory evolution and accumulation maps of re-solidified droplets.
D8	Prediction of fuel inventory in multi-component PFC including thermal and mechanical effects, accounting for neutron and He damage, morphological changes.
D9	Uptake of D/T in W and across interfaces to the coolant and respective UQ.
D10	Fully kinetic sheath simulations in 1D/3D providing plasma profiles and boundary conditions at the plasma sheath based on the DEMO plasma solution.
D11	Effective W erosion yields for rough surfaces and re-solidified melt layers, including UQ.
D12	W erosion yields under D/T supersaturation as function of ion impact energies, angles, and surface temperature.
D13	W-O and W-O-H interatomic potentials.
D14	A suite of HPC optimized codes for DEMO PWI with IMAS-adapted data exchange.

Timeline


2021
2022
2023
2024
2025
Plasma
ITER bg proc.
DEMO bg proc.
VDE, LOC values
VDE, LOC profiles
Updates from DEMO team:
geometry, materials, plasma profiles
PIC
Sheath ion distrib.
Gaps
Thermionic & SEE
BIT3 vs BIT1
PWI 1
W erosion under D/T supersaturation
W-O-H potential
W-O potential
PWI2
Gyromotion
SDTrimSP-3D
UQ interface
UQ studies
ERO2.0
Preps (geom., bg)
Deposition in gaps
Simulations ITER-like
SDTrimSP-1D coupling
Simulations DEMO
SDTrimSP-3D data and coupling
Fuel retention
Thermomigration
Simulations DEMO
Simulations DEMO
He (H diffusion)
He (W mechanical)
Interface model
w/o n-damage
with n-damage
Test cases
UQ interface
UQ studies
Transient melting
Preps
Melting, splashing
Dust
Scoping studies
Simulations DEMO steady
Simulations ITER-like
Simulations DEMO transients
Report DEMO CDR
Final report

Communication

Task progress and completion will be monitored, evaluated and documented. Regular group and team meetings and information exchange will be organized as summarized below.

Communication goal	*Format*	*Audience*	*Frequency*
Information exchange, clarification of ongoing issues	E-mail / In-person / VC	Various team members	On demand
Group stand-up meetings	In-person / VC	Sub-teams	On demand
Coordination meetings	VC	Task leader, sub-task leaders	Monthly (on demand)
Team stand-up meetings	VC	Full team	Every 2 months
Task progress meeting	In-person / VC	Full team	Yearly
Interim reporting meeting for DEMO CDR	In-person / VC	Full team, E-TASK scientific board	2023/24
Final reporting meeting	In-person / VC	Full team, E-TASK scientific board	2025/26

ACH Support

- 5 Advanced Computer Hubs:

Category 1. High Performance Computing [edit]

(scalable algorithms, code parallelization & performance optimization, code refactoring, GPU-enabling etc.)

ACH-01: *MPG*	Roman Hatzky
ACH-02: *EPFL*	Paolo Ricci
ACH-03: *CIEMAT*	Mervi Mantsinen

Category 2. Integrated Modelling and Control [edit]

(code adaptation to IMAS, IMAS framework development, code integration etc.)

ACH-04: *IPPLM*	Marcin Plociennik

Category 3. Data management [edit]

(open access, data management, data analysis tools, aspects of AI and VVUQ etc.)

ACH-05: *VTT*	Fredric Granberg

ACH Support

- 5 Advanced Computer Hubs:

IMAS is installed in most EUROfusion experimental sites

ACH will take the charge of supporting installation of IMAS to additional clusters or HPCs specified by the TSVVs

There is a contenerised/dockerised version of the IMAS developed at IPPLM with usage of the udocker and some use cases on Marconi and in other HPCs like in BSC

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ACH Support

- Requests for ACH support (by April,15)

Code name	Tasks required to ACH
BIT-1	?
BIT-3	?
SPICE-2	Upscaling from cluster-parallel to HPC-parallel
SPICE-3	
ERO2.0	Improved parallelization (e.g. compiler opt, GPU)
MEMOS-U	Improvement of the code architecture and modularity, reduction of memory consumption
MIGRAINe	HPC compatibility of the effective parallelization
SDTrimSP-1D	?
SDTrimSP-3D	?
RAVETIME	Upscaling from cluster-parallel to HPC-parallel
Interatomic potentials	Optimization and GPU-enabling
Retention codes	?

Marconi 5th Fusion cycle

Following the evaluation process

the project TSVV7 was allocated:

- 307 200 node-h (~60% of requested)

  to run on the A3 conventional partition

  - To be used by

    BIT1

    SPICE1D/2D/3D

    ERO2.0

    MEMOS-U

Project: EUROfusion A3 Phase 5

AccountID: TSVV7

Science Domain: Nuclear Fusion

Validity: Monday, 1 March, 2021 to Monday, 28 February, 2022

Status:

Active

ExpirationDelay:

6

Details

Hosts: MARCON3

Budget (standard hours): 307 200

WORK Quote (in GB): 1 024

Online resources

- Wiki-pages for Advanced Computing (WPAC) – working space for projects

  https://wiki.euro-fusion.org/wiki/WPAC_wikipages:_Advance_Computing_Work_Package

  https://wiki.euro-fusion.org/wiki/TSVV-07

- INDICO – meeting organization and presentation storage

  https://indico.euro-fusion.org/category/209/

- IMAS sources of information
  - Integrated modelling homepage (ITER account required)

    https://confluence.iter.org/display/IMP

  - Tutorials from the Polish group

    https://confluence.man.poznan.pl/community/display/WFMS/ITER

Kick-Off Meeting

- TSVV/ACH Kick-Off Meeting will take place on 23.04.2021 for (PIs only)
  - Program available in INDICO
    - 10-min introduction of each Thrust and ACH: organization and key objectives
    - 40-min parallel sessions: free-format discussions on objectives and interactions in Thrusts
    - Wrap-up session: a brief summary of each parallel session
- TSVV7 Kick-Off Meeting to take place in the beginning of May (open for public?)
  - One presentation per sub-task introducing the tools, current state, dependencies/requirements
  - Detailing the work plan for 2021
  - Planning interactions with ACHs (to be boosted in 2021)